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Titolo	Computational modeling for homogeneous and enzymatic catalysis [[electronic resource]] : a knowledge-base for designing efficient catalysts / / edited by Keiji Morokuma and Djamaladdin G. Musaev
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Altri autori (Persone)	MorokumaK <1934-> (Keiji) MusaevDjamaladdin G
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Soggetti	Catalysis - Computer simulation Catalysts Electronic books.
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Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Computational Modeling for Homogeneous and Enzymatic Catalysis; Contents; Preface; List of Contributors; 1 Computational Insights into the Structural Properties and Catalytic Functions of Selenoprotein Glutathione Peroxidase (GPx); 1.1 Introduction; 1.2 Catalytic Functions; 1.2.1 Peroxidase Activity; 1.2.2 Reductase Activity; 1.3 Computational Details; 1.3.1 Computational Methods; 1.3.2 Computational Models; 1.4 Results and Discussion; 1.4.1 Refinement of the Active Site; 1.4.2 Catalytic Functions: Peroxidase Activity 1.4.3 Catalytic Functions: Effect of the Surrounding Protein on the Peroxidase Activity 1.4.3.1 Hydrogen Peroxide Coordination; 1.4.3.2 Formation of Selenenic Acid [E-Se-OH]; 1.4.4 Catalytic Functions: Reductase Activity; 1.4.4.1 Peroxynitrite/Peroxynitrous Acid (ONOO /ONOOH) Coordination; 1.4.4.2 Oxidation Pathway; 1.4.4.3 Nitration Pathways; 1.5 Summary; References; 2 A Comparison of Tetrapyrrole Cofactors in Nature and their Tuning by Axial Ligands; 2.1 Introduction;

2.2 Methodology; 2.3 Comparison of the Intrinsic Chemical Properties of the Tetrapyrroles; 2.3.1 Introduction
2.3.2 Spin States
2.3.3 Tetrapyrroles Prefer Their Native Ions; 2.3.4 Cavity Size and Flexibility of the Tetrapyrroles; 2.3.5 Cytochrome-like Electron Transfer; 2.3.6 Stability of a Metal-Carbon Bond; 2.3.7 Metallation Reaction; 2.4 Tuning of Tetrapyrrole Structure and Function by Axial Ligands; 2.4.1 Introduction; 2.4.2 Importance of the Lower Axial Ligand for B(12) Chemistry; 2.4.3 Lower Axial Ligand in Cofactor F430; 2.4.4 Importance of Axial Ligands for the Globins; 2.4.5 Role of Axial Ligands for the Cytochromes; 2.4.6 Role of the Axial Ligand in Heme Enzymes
2.4.7 Tuning the His Ligand by Hydrogen Bonds in Heme Proteins
2.4.8 Axial Ligand in Chlorophylls; 2.5 Concluding Remarks; References; 3 Modeling of Mechanisms for Metalloenzymes where Protons and Electrons Enter or Leave; 3.1 Introduction; 3.2 Energy Diagrams; 3.2.1 Photosystem II; 3.2.2 Cytochrome c Oxidase; 3.2.3 Nitric Oxide Reduction; 3.2.4 NiFe-hydrogenase; 3.2.5 Molybdenum CO Dehydrogenase; 3.3 Conclusions; References; 4 Principles of Dinitrogen Hydrogenation: Computational Insights; 4.1 Introduction
4.2 Reaction Mechanism of the Coordinated Dinitrogen Molecule in Di-zirconocene-N(2) Complexes with a Hydrogen Molecule
4.2.1 Mechanism of the Reaction (3); 4.2.2 Mechanisms of the Reactions (4) and (5); 4.3 Factors Controlling the N(2) Coordination Modes in the Di-zirconocene-N(2) Complexes; 4.4 Why the $[(\eta^5\text{-C}_5\text{Me}_n\text{H}_{5-n})_2\text{Ti}](\eta^2)(\eta^2)(\eta^2)\text{-N}_2$ Complex Cannot Add a H(2) Molecule to the Side-on Coordinated N(2), while its Zr- and Hf-analogs Can
4.4.1 Relative Stability of the Lowest Singlet (S) and Triplet (T) Electronic States of the Complexes $[(\eta^5\text{-C}_5\text{Me}_n\text{H}_{5-n})_2\text{M}](\eta^2)(\eta^2)(\eta^2)\text{-N}_2$, II_M (for M = Ti, Zr, and Hf, and n = 0 and 4)

Sommario/riassunto

Here, the world's most active and productive computational scientists from academia and industry present established, effective and powerful tools for understanding catalysts. With its broad scope -- nitrogen fixation, polymerization, C-H bond activation, oxidations, biocatalysis and much more -- this book represents an extensive knowledge base for designing efficient catalysts, allowing readers to improve the performance of their own catalysts.

2. Record Nr.	UNINA9910633937003321
Autore	Wybraniec-Skardowska Urszula
Titolo	Logic - Language - Ontology : Selected Works // by Urszula B. Wybraniec-Skardowska
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ISBN	9783031223303 9783031223297
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Descrizione fisica	1 online resource (305 pages)
Collana	Studies in Universal Logic, , 2297-0290
Disciplina	401
Soggetti	Mathematics - Philosophy Logic, Symbolic and mathematical Logic Set theory Philosophy of Mathematics Mathematical Logic and Foundations Formal Logic Philosophical Logic General Logic Set Theory
Lingua di pubblicazione	Inglese
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Nota di bibliografia	Includes bibliographical references.
Nota di contenuto	Part I Introduction -- 1. The Dual Ontological Nature of Language Signs and the Problem of Their Mutual Relations -- 2 On the Structure and Contents of the Monograph -- Part II SelectedWorks -- 1. On the Type-Token Relationships -- 2. On the Axiomatic Systems of Syntactically-Categorical Languages -- 3. The Logical Foundations of Language Syntax Ontology -- 4. On the Eliminatibility of Ideal Linguistic Entities -- 5. Meaning and Interpretation. Part I -- 6. Meaning and Interpretation. Part II -- 7. Three Principles of Compositionality -- 8. On Meta-knowledge and Truth -- 9. On Language Adequacy -- 10. What Is the Sense in Logic and Philosophy of Language? -- 11. Categories of First-Order Quantifiers -- 12. Logic and the Ontology of Language -- 13. A Logical Conceptualization of Knowledge on the

Notion of Language Communication.

Sommario/riassunto

How should we think about the meaning of the words that make up our language? How does reference of these terms work, and what is their referent when these are connected to abstract objects rather than to concrete ones? Can logic help to address these questions? This collection of papers aims to unify the questions of syntax and semantics of language, which span across the fields of logic, philosophy and ontology of language. The leading motif of the presented selection is the differentiation between linguistic tokens (material, concrete objects) on the one hand and linguistic types (ideal, abstract objects) on the other. Through a promenade among articles that span over all of the Author's career, this book addresses the complex philosophical question of the ontology of language by following the crystalline conceptual tools offered by logic. At the core of Wybraniec-Skardowska's scholarship is the idea that language is an ontological being, characterized in compliance with the logical conception of language proposed by Ajdukiewicz. The application throughout the book of tools of classical logic and set theory results fosters the emergence of a general formal logical theory of syntax, semantics and of the pragmatics of language, which takes into account the duality token-type in the understanding of linguistic expressions. Via a functional approach to language itself, logic appears as ontologically neutral with respect to existential assumptions relating to the nature of linguistic expressions and their extra-linguistic counterparts. The book is addressed to readers both at the graduate and undergraduate level, but also to a more general audience interested in getting a firmer grip on the interplay between reality and the language we use to describe and understand it.